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#### ECI 2015 - Buenos Aires T3: Symbolic Data Analysis: Taking Variability in Data into Account





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# Principal Component Analysis: Objectives

Principal Component Analysis applies to data described by  $(p)$ numerical variables.

Objective:

to obtain an approximate representation of the individuals in a sub-space of dimension  $q < p$ .

That is, to represent them with a small set of variables

The representation in a space of lower dimension is done by a projection - and NOT by variable selection.

→ Dimension reduction

 $\mathcal{A} \xrightarrow{\sim} \mathcal{B} \rightarrow \mathcal{A} \xrightarrow{\sim} \mathcal{B} \rightarrow$ 

### Principal Component Analysis: Objectives

The choice of the new representation space is done according to the following criterion :

The average squared distance between projected points (measuring their dispersion) must be as large as possible.

We wish to distort the point configuration as little as possible and therefore also the distances between them (they can only decrease).

In other words:

the dispersion of the projected point set should be maximized

# Principal Component Analysis: Objectives

From the variables point of view,

the problem consists in determining new variables linear combinations of the original variables (previously centered) non-correlated among themselves, and with maximum variance

The solution is nested :

The best subset of  $q$  (new) variables is obtained from the best subset of  $q - 1$  variables,

together with the best aditional variable, non-correlated with them, that maximizes the dispersion in the projection.

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### Principal Component Analysis: Solution

The solution of the problem is given by the  $(q)$  normed eigenvectors of the variance-covariance matrix V, in non-normed PCA

or of the correlation matrix R, in normed PCA associated to the  $(q)$  largest eigenvalues

$$
\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_q
$$

The total dispersion of the projected dataset

 $=$  sum of the variances of the new variables is given by:



#### Principal Component Analysis: Properties

- The principal components are variables with null mean
- The principal components are non-correlated variables
- The variance da  $\alpha_{th}$  principal component  $c_{\alpha}$  is equal to the correponding eigenvalue
- The principal components are linear combinations of the centered (or standardized) original variables, defined by the eigenvectors associated with the corresponding eigenvalues

If an important part of the dispersion is explained by a small number  $q$  of principal components:

we may use just some of them for interpretation and future analysis, instead of the original  $p$ 

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- Factorial method for interval data
- Graphical representation by rectangles in the factorial planes
- **·** Interpetation indices

Direct solution:

- $\bullet$  use covariance / correlation values obtained for the interval-valued variables
- proceed as for real (classical) data
- obtain interval representations in the new variables' space applying the linear combinations to lower and upper bounds of the observed data

Two first methods

(Cazes, P., Chouakria, A., Diday, E., Schektman, Y. (1997)) :

- Vertices method: Analysis of the data array with  $n \times 2p$  rows and p coloumns containing all vertices of the hyper-rectangles in the interval data-array
- **C**entres method:

Replaces each interval by its centre

See also: Chouakria, A., Billard, L., Diday, E. (2011)

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Example:

if  $s_i$  has the description ([a, b], [c, d]),  $s_i$  will be "transformed" in :

$$
\left[\begin{array}{ccc} a & c \\ b & c \\ a & d \\ b & d \end{array}\right]
$$

A classical PCA of the new  $(n \times 2p)$  rows  $\times p$  columns data array is performed.

Weight of 
$$
s_i = \frac{p_i}{2^p} (p_i : original weight of s_i)
$$

<span id="page-13-0"></span>Let  $Y^*_j$  be the les  $q$  first principal components,  $j=1,\ldots,q$ 

For each principal component  $Y_j^*$ :

the minimum value  $min_i(s_i)$  and the maximum value  $max_i(s_i)$  of  $Y_j^*$  are detemined, accross the 2p rows representing each entity  $s_i$ 

We then define:  $Y_j^*(s_i) = [min_j(s_i), max_j(s_i)]$ 

<span id="page-14-0"></span>Interpretation indices: Quality of representation

- G : centre of gravity of the  $n \times 2p$  points
- d : Euclidean distance
- $L_i$ : 2p points representing  $s_i$

Contribution of the 2p vertices representing  $s_i$  to the total sum of squares:

$$
COR^{1}(i, v_{j}) = \frac{\sum_{k \in L_{i}} Y_{kj}^{*2}}{\sum_{k \in L_{i}} d^{2}(k, G)}
$$

Mean of the squared cossinus of the angles between the  $2p$  vertices representing  $s_i$  and the factorial axis  $v_j$ :

$$
COR^2(i, v_j) = \frac{1}{2^p} \frac{\sum_{k \in L_i} Y_{kj}^{*2}}{\sum_{k \in L_i} d^2(k_{\overline{y}} \mathbf{G}) \mathbf{G} \mathbf{G} \mathbf{G} \mathbf{G}}
$$

### <span id="page-15-0"></span>Interpretation indices: Contributions

Contribution of  $s_i$  to the variance of the  $j^{th}$  principal component:

$$
CTR(i, v_j) = \frac{\sum_{k \in L_i} q_k Y_{kj}^{*2}}{\lambda_j} = \frac{p_i}{2^p \lambda_j} \sum_{k \in L_i} Y_{kj}^{*2}
$$

Contribution of  $s_i$  to the total inertia:

$$
INR(i) = \frac{p_i}{2^p} \frac{\sum_{k \in L_i} d^2(k, G)}{\sum_j \lambda_j}
$$

# SPCA: Centres method

Only the intervals' midpoints are used.

Example:

if  $s_i$  has the description ([a, b], [c, d]),  $s_i$  will be "transformed" in :

$$
c_i = \left(\frac{a+b}{2}, \frac{c+d}{2}\right)
$$

A classical PCA of the new  $n \times p$  data array is performed

$$
x_{ij}^c
$$
: midpoint of variable  $Y_j$  for entity  $s_i$  (centre  $c_i$ )

 $\overline{\mathsf{x}_{j}^{\mathsf{c}}}$  : mean of the midpoints of variable  $\mathsf{Y}_{j}$ 

$$
v_{\ell} = (v_{1\ell}, \ldots, v_{p\ell}) : \text{ the } \ell^{\text{th}} \text{ eigenvector}
$$

The  $\ell^{th}$  principal component of centre  $c_i$  is given by:

$$
Y_{i\ell}^{*c} = \sum_{i=1}^{p} (x_{ij}^{c} - \overline{x_{j}^{c}}) v_{j\ell}
$$
  
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# SPCA: Centres method

 $I_{ii}$ : interval corresponding to entity  $s_i$  and variable  $Y_i$ 

Interval corresponding to  $s_i$  for the  $\ell^{th}$  principal component:

$$
I_{ij}^* = [I_{ij}^*, \overline{I_{ij}^*}]
$$

$$
I_{ij}^* = \sum_{j=1}^p \text{Min}_{x \in I_{ij}} \{ (x - \overline{x_j^c}) v_{j\ell} \}
$$

$$
\overline{I_{ij}^*} = \sum_{j=1}^p \text{Max}_{x \in I_{ij}} \{ (x - \overline{x_j^c}) v_{j\ell} \}
$$

 $\left\{ \begin{array}{ccc} \pm & \pm & \pm & \pm & \pm \end{array} \right.$ 

[Introduction to PCA](#page-2-0) [Principal Component Analysis for Interval Data](#page-8-0)

### Principal Component Analysis of Interval data



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<span id="page-19-0"></span>Other methods for PCA of Interval data:

- Lauro, C., Palumbo, F. (2000). Principal component analysis of interval data:a symbolic data analysis approach.
- Palumbo, F., Lauro, C. (2003). A PCA for interval valued data based on midpoints and radii.
- Gioia, F., Lauro, C. (2006). Principal component analysis on interval data.
- Irpino, A. (2006). "Spaghetti" PCA analysis: An extension of principal component analysis to time dependente interval data.